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## Modeling geometric arrangements of TiO<sub>2</sub>-based catalyst substrates and isotropic light sources to enhance the efficiency of a photocatalytic oxidation (PCO) reactor

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The closed confined environments of the ISS, as well as in future spacecraft for exploration beyond LEO, provide many challenges to crew health. One such challenge is the availability of a robust, energy efficient, and re-generable air revitalization system that controls trace volatile organic contaminants (VOCs) to levels below a specified spacecraft maximum allowable concentration (SMAC). Photocatalytic oxidation (PCO), which is capable of mineralizing VOCs at room temperature and of accommodating a high volumetric flow, is being evaluated as an alternative trace contaminant control technology. In an architecture of a combined air and water management system, placing a PCO unit before a condensing heat exchanger for humidity control will greatly reduce the organic load into the humidity condensate loop of the water processing assembly (WPA) thereby enhancing the life cycle economics of the WPA. This targeted application dictates a single pass efficiency of greater than 90% for polar VOCs. Although this target was met in laboratory bench-scaled reactors, no commercial or SBIR-developed prototype PCO units examined to date have achieved this goal. Furthermore, the formation of partial oxidation products (e.g., acetaldehyde) was not eliminated. It is known that single pass efficiency and partial oxidation are strongly dependent upon the contact time and catalyst illumination, hence the requirement for an efficient reactor design. The objective of this study is to maximize the apparent contact time and illuminated catalyst surface area at a given reactor volume and volumetric flow. In this study, a TiO<sub>2</sub>-based photocatalyst is assumed to be immobilized on porous substrate panels and illumination derived from linear isotropic light sources. Mathematical modeling using computational fluid dynamics (CFD) analyses were performed to investigate the effect of: 1) the geometry and configuration of catalyst-coated substrate panels, 2) porosity of the supporting substrate, and 3) varying the light source and spacing on contact time and illuminated catalyst area.